Heptafluorobutyric acid 375-22-4 | DTXSID4059916

Model Performance

| Model | Data |
|---------|------|
| iviodei | Dala |

Weighted KNN model

| 5-fold CV (| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-------------|-----------------|------|----------------|------|------------|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 | |

Model Results

Predicted value: 2.31

Global applicability domain: Inside

Local applicability domain index: 4.83e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl perfluoropropionate

Measured: 2.12 Predicted: 2.04

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1-Butanol, 2,2,3,3,4,4,4-

heptafluoro-Measured: 1.94 Predicted: 1.93

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1-Hexanol, 3,3,4,4,5,5,6,6,6-

nonafluoro-**Measured:** 3.30 **Predicted:** 3.01